2,2'-Dihydroxybenzophenone 835-11-0 | DTXSID8022404

Model Performance

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | | |
|-----------------|------|----------------|------|------------|------|--|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE | |
| 0.93 | 22.5 | 0.93 | 22.1 | 0.93 | 22.1 | |

Model Results

Predicted value: 318 °C

Global applicability domain: Inside

Local applicability domain index: 3.26e-01

Confidence level: 6.66e-01

Nearest Neighbors from the Training Set

Image not found

2,2'-Dihydroxybenzophenone

Measured: 333 Predicted: 318

Image not found

(1,1'-Biphenyl)-2,2'-diol

Measured: 320 Predicted: 315

Image not found

4-Hexylresorcinol Measured: 334 Predicted: 302

Image not found

tert-Butylhydroquinone

Measured: 273 Predicted: 277

Image not found

4-tert-Butylcatechol Measured: 285 Predicted: 277